

# **Applications of Automatic Differentiation**

**Lawrence L. Green**

**Multidisciplinary Optimization Branch**

**Aerospace Concepts and Analysis Competency**

**Methods Development Peer Review - Nov. 2001**

## **Current Collaborators:**

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**2 NASA LaRC / AAAC / CMSB**

**3 Boeing Long Beach**

**4 NASA LaRC / AirSC / DCB**

**5 NASA LaRC / ASCAC / MDOB**

**6 NASA LaRC / AirSc / VDB**

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# ASCoT Project (1998-2002)

## (Aerospace Systems Concept to Test)

### Project Vision

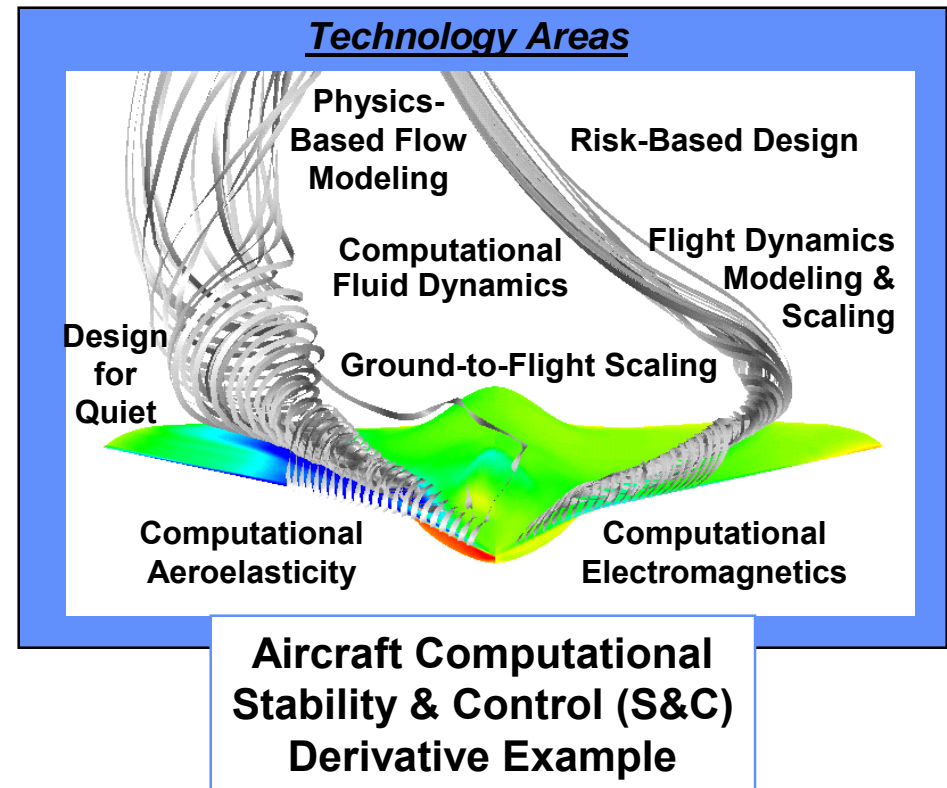
*Physics-based modeling and simulation with sufficient speed and accuracy for validation and certification of advanced aerospace vehicle design in less than 1 year*

### Project Goal

- Provide **next-generation analysis & design tools** to increase confidence and reduce development time in aerospace vehicle designs

### Objective

- Develop **fast, accurate, and reliable** analysis and design tools via fundamental technological advances in:
  - **Physics-Based Flow Modeling**
  - Fast, Adaptive, Aerospace Tools (CFD)
  - Ground-to-Flight Scaling
  - **Time-Dependent Methods**
  - Design for Quiet
  - **Risk-Based Design**



### Benefit

- Increased Design Confidence
  - Reduced Development Time
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# Introduction to Sensitivity Methods

## Motivation / Objectives

- Accurate and consistent derivatives of disciplinary analyses are needed for optimization and uncertainty analyses
- Legacy analysis codes don't usually provide derivatives
- Respond quickly to changes in the design environment
  - Design variables, objective, and constraints
  - Algorithms, physics models, and computational paradigms
- Sensitivity methods
  - + physics-based flow modeling = **static S&C derivatives**
  - + time dependent methods = **dynamic S&C derivatives**
  - + optimization methods = **conventional design**
  - + uncertainty propagation = **robust design**
- Assess / improve the computational impact
- Transfer tools and techniques to others

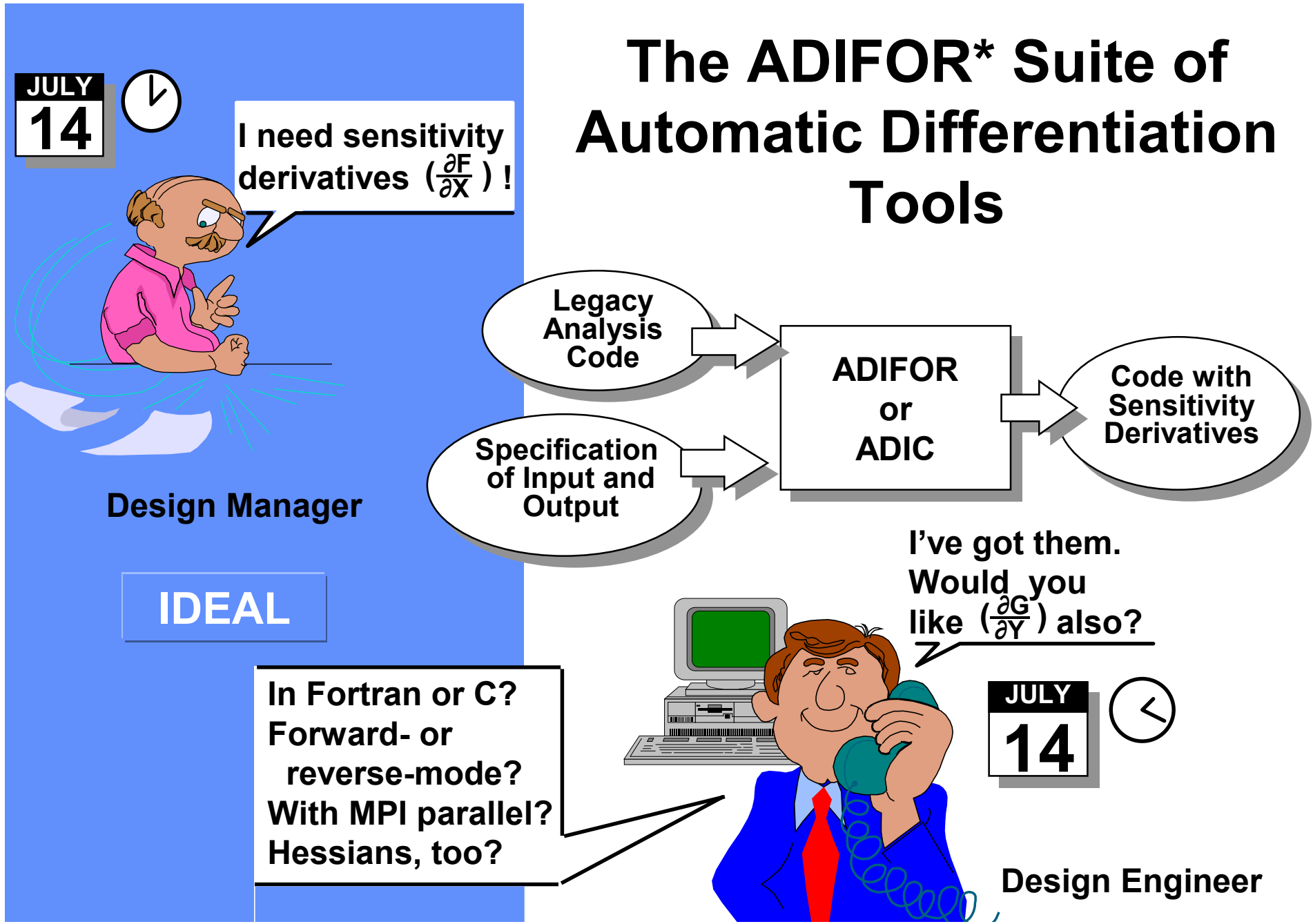
# Introduction to Sensitivity Methods

## Comparison of Methods

- Finite-differences (FD) (approximation, step size dependent)
- Manual differentiation (exact, tedious, prone to errors)
- Symbolic manipulators (exact, limited scope of application)
- Complex arithmetic (exact, similar to FD, can't be used if complex arithmetic is already present, no adjoint formulation)
- **Automatic Differentiation (AD) – ADIFOR**
  - Application is fast and easy for standard Fortran 77
  - Exact to machine and problem formulation precision
  - Can be computationally much faster than FD
  - Forward (direct) and reverse (adjoint) forms available
  - Rigorous verification of accuracy (not discussed here)
- Hybrid schemes (AIAA 94-4262\* and AIAA 2001-2529)
  - Leverage strengths / minimize weaknesses of several methods
  - Employ disciplinary, code, and differentiation knowledge
  - Improve computational efficiency

\* Also, Journal of Computational Physics, Vol. 129, p307-331, 1996

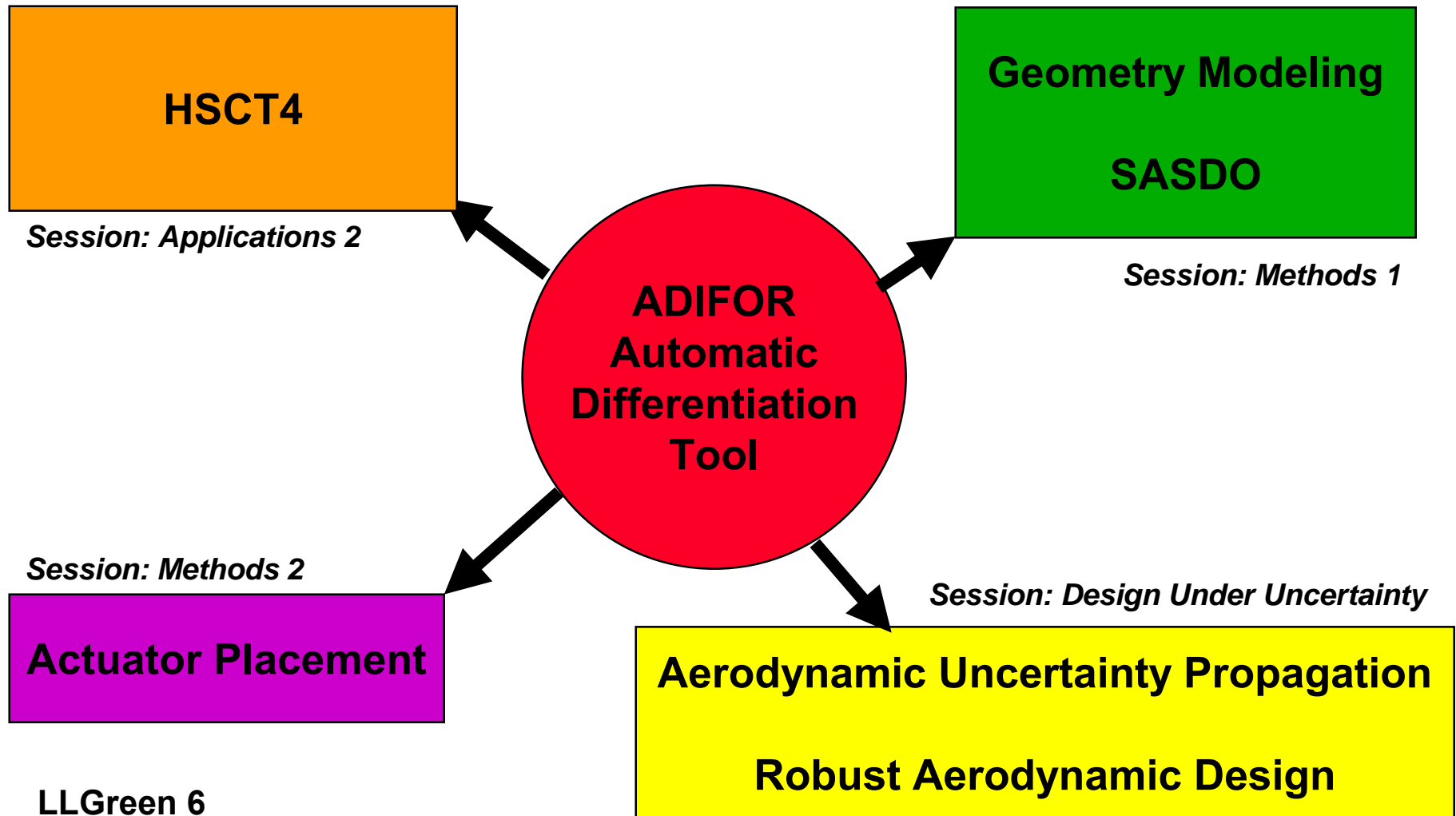
# The ADIFOR\* Suite of Automatic Differentiation Tools



\* Developed by Rice University and Argonne National Laboratory  
Winner 1995 Wilkinson Prize for Numerical Software

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# ADIFOR Connections to Other MDOB Activities



# PMARC

- Panel Method – Ames Research Center
- Dale Ashby, et.al. (NASA ARC)
- Time-dependent low-order potential-flow with boundary-layer correction
- Forward- and reverse-mode ADIFOR applications

# CFL3D

- Computational Fluids Laboratory 3-Dimensional
- Thomas, Rumsey, Biedron, etc. (NASA LaRC)
- Euler / Navier-Stokes (N-S); several turbulence models
- N-S Spalart-Allmaras (S-A) turbulent flow cases presented
- Executes on NASA Langley and Ames Silicon Graphics, Inc.(SGI) Origin 2000™ parallel computers
- Version 6 includes dynamic memory and MPI parallel execution
- Version 6+ modified for steady-state, constant rotational rate motions

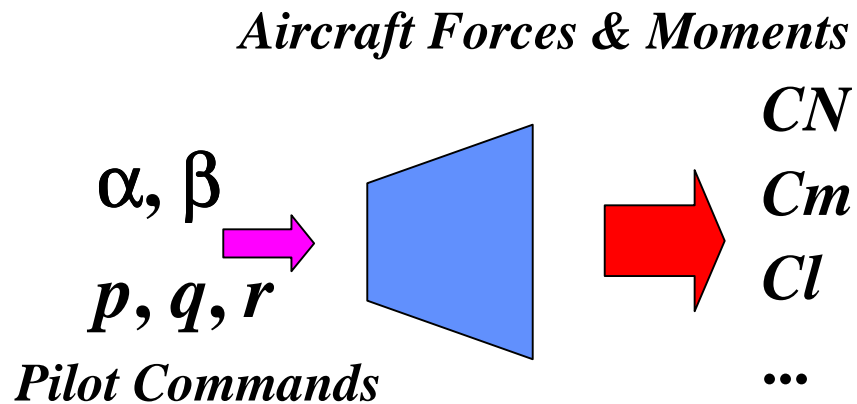
# Featured ADIFOR 3.0 Applications

- Computation of static / dynamic stability and control derivatives
  - 5 control variables / 6 aircraft responses
  - Forward mode AD application to PMARC and CFL3D
  - MDOB, AirSC/VDB, AirSC/DCB, and Lockheed-Martin (1998 - 2000)
- High Speed Civil Transport aerodynamic shape optimization
  - 401 design variables / 56 constraints / 1 aircraft response
  - Reverse-mode AD application to CFL3D
  - Boeing Long Beach with MDOB expertise (1999 - 2000)
- Reusable Launch Vehicle (RLV) aero-thermal shape optimization
  - 35 design variables / 6 constraints / 2 vehicle responses
  - Reverse-mode AD application to CFL3D with thermal effects
  - Boeing Long Beach with MDOB funding and expertise (2001)
- Control placement effectiveness study (time permitting)
  - 1353 placement variables / 3 aircraft responses
  - Reverse-mode AD application to PMARC
  - MDOB, AirSC/DCB, and Lockheed-Martin (1998)

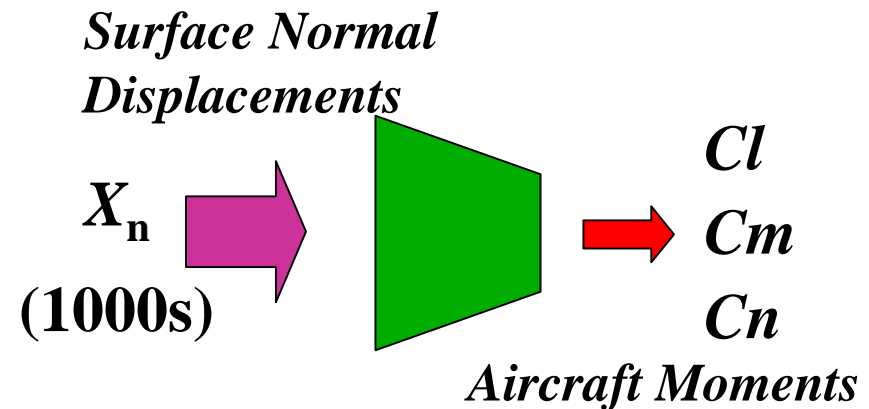


# Example ADIFOR Applications

- CFL3D Euler/Navier-Stokes code
- **Forward** mode
- Chain rule of calculus
- Number of variables:  
**dependent** > **independent**
- Aircraft stability derivatives
- PMARC linear aerodynamics code
- **Reverse** Mode
- Discrete adjoint formulation
- Number of variables:  
**independent** > **dependent**
- Control placement effectiveness

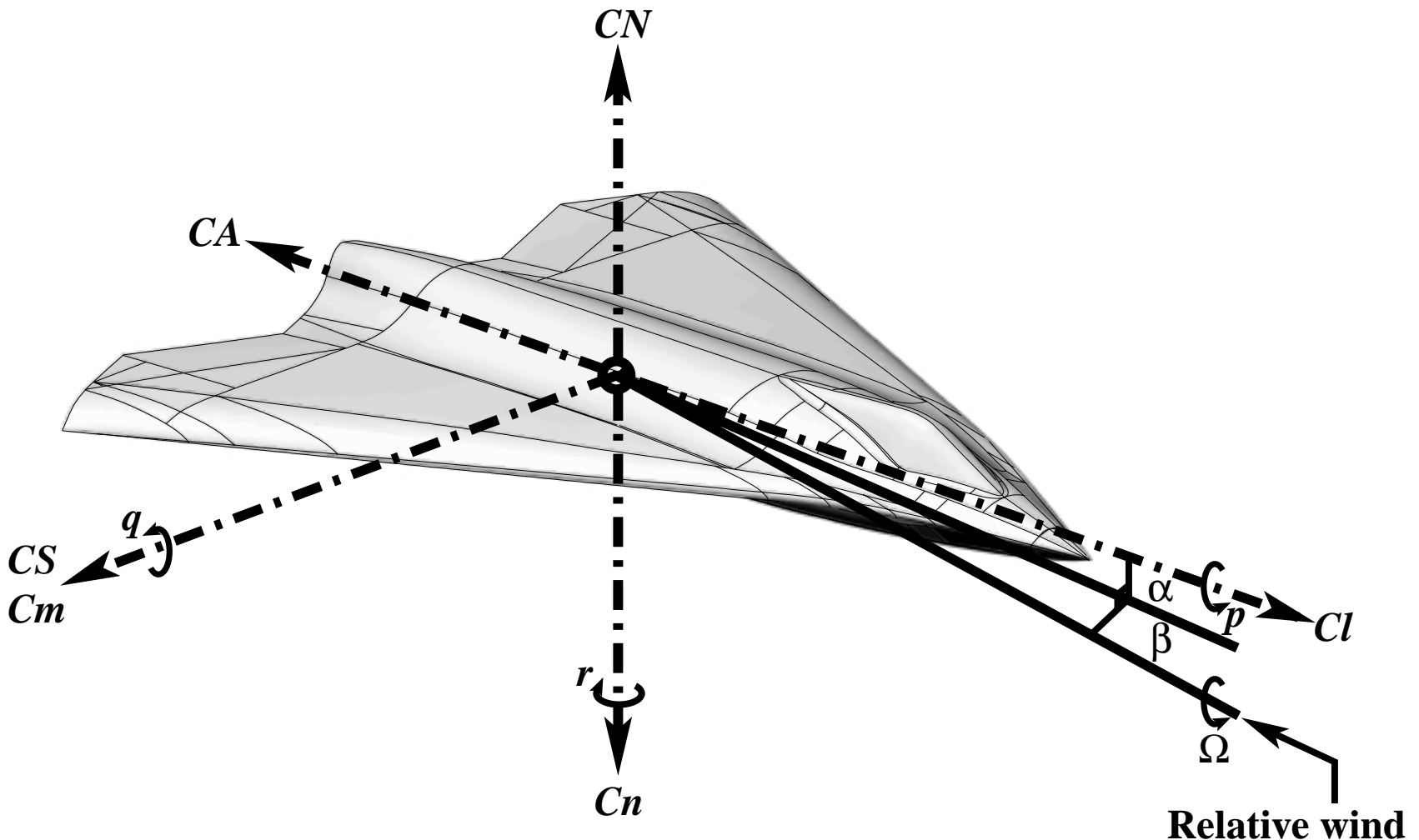


AIAA 99-3136  
AIAA 2000-4321



AIAA 98-4807  
AIAA 2000-1560

# Lockheed-Martin Innovative Control Effectors (ICE) Configuration

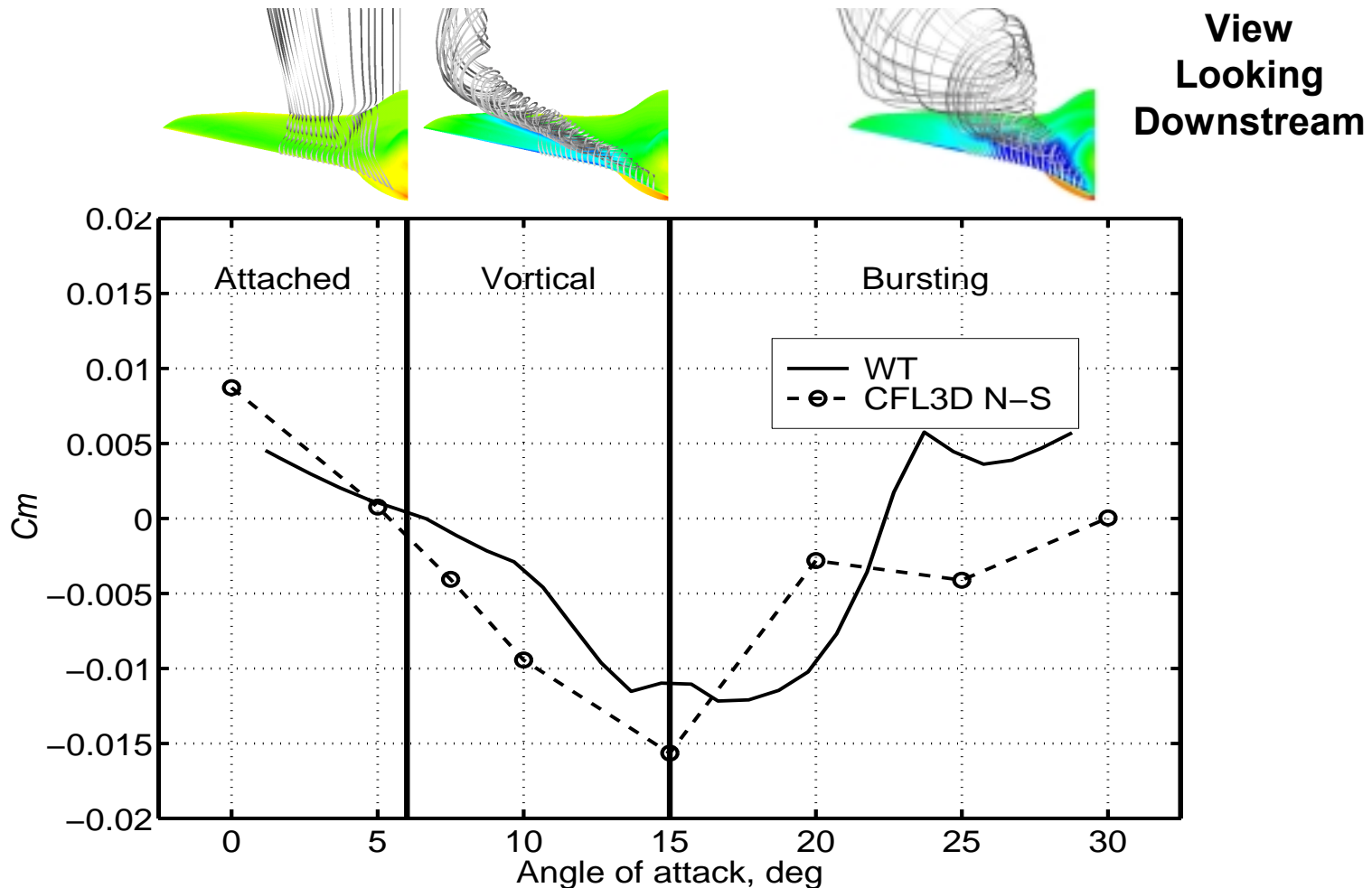


CFD volume grid 3 with million cells, full span  
and derived linear aerodynamics surface grid

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# Three $\alpha$ ranges of flow structure

Pitching Moment, CFL3Dv6 N-S S-A, Mach = 0.6, ICE Configuration



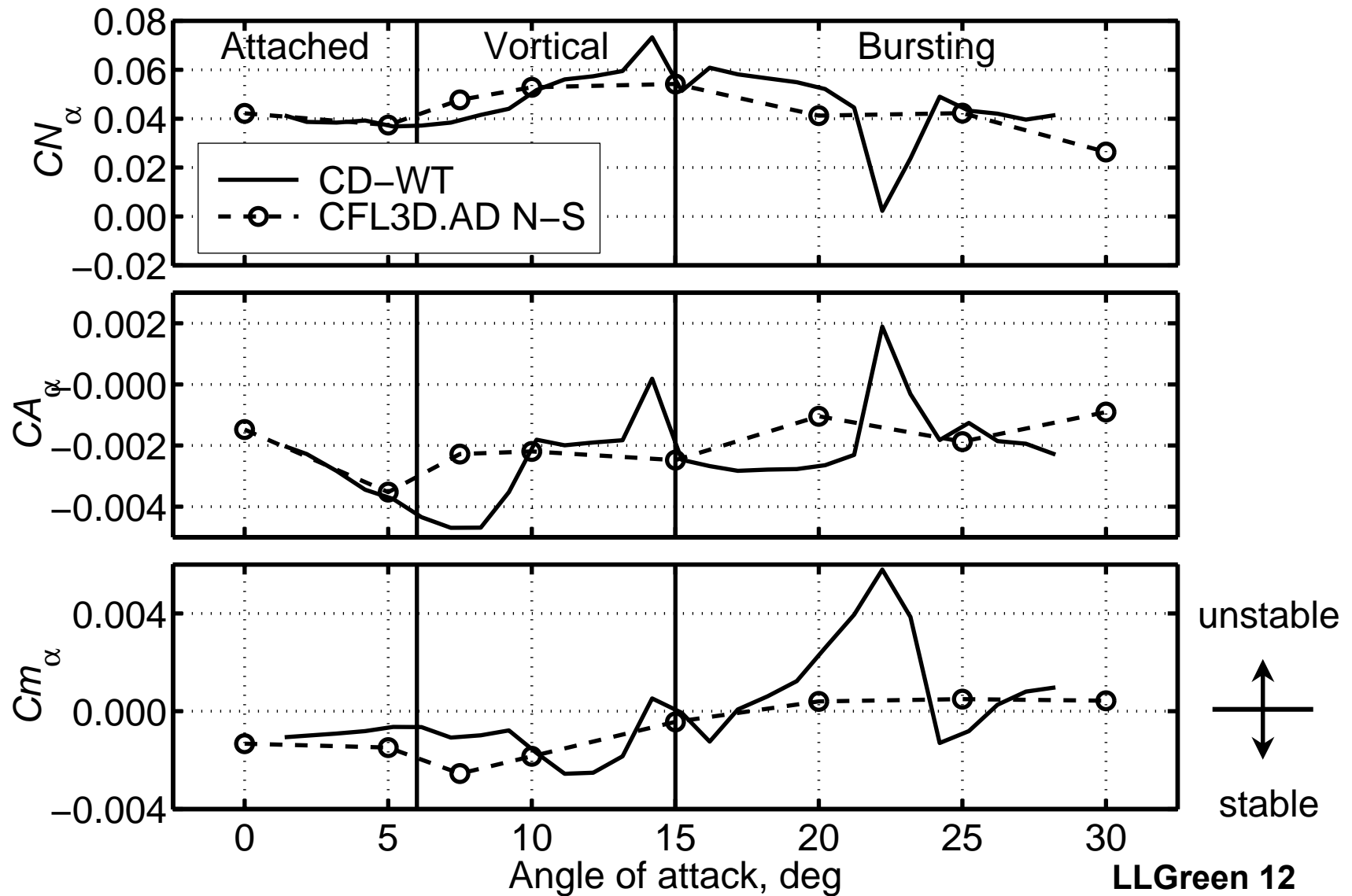
Angle of attack resolution: WT (~1 deg), CFD (~5 deg)

Good agreement for CN and CA with WT

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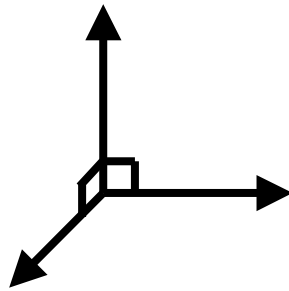
# Long. Static Stability ( $\alpha$ derivatives)

CFL3Dv6.AD N-S / S-A, Mach = 0.6, ICE Configuration

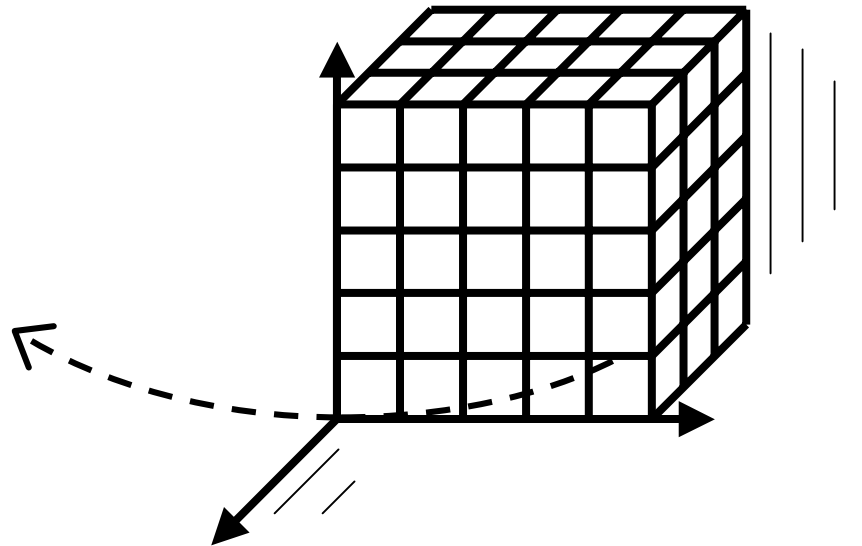


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# Non-inertial Frame of Reference<sup>1</sup>



**Inertial (fixed)**



**Non-inertial CFD grid (moving)**

- Efficient method to simulate moving CFD grids
  - Steady-state solutions of constant-rate motion
- Relatively simple to implement
  - Add source term to governing equations (induced body forces)
  - Increment boundary and initial conditions (rotational velocities)

<sup>1</sup> Limache, A. C. and Cliff, E. M.: "Aerodynamic Sensitivity Theory for Rotary Stability Derivatives", AIAA 99-4313

# Non-inertial Modifications to CFL3Dv6

Solution update:  $\frac{1}{J} \frac{\partial Q}{\partial t} = R(Q) + S$  **Source Term**

Conserved  
variables:

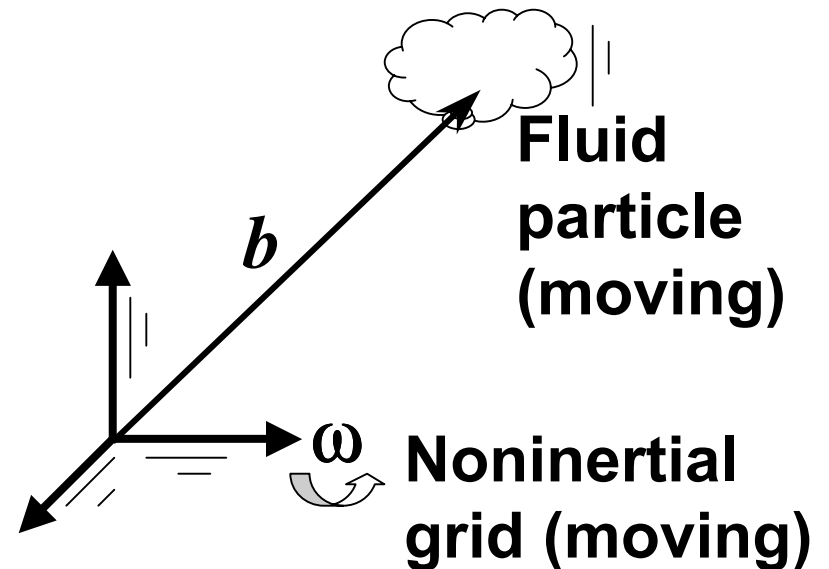
$$Q = [\rho \quad \rho u \quad \rho v \quad \rho w \quad e]^T$$

Source term:

$$S = \frac{\rho}{J} \begin{bmatrix} 0 & \bar{\Theta}_x & \bar{\Theta}_y & \bar{\Theta}_z & \bar{\Theta}_g \end{bmatrix} b^T$$

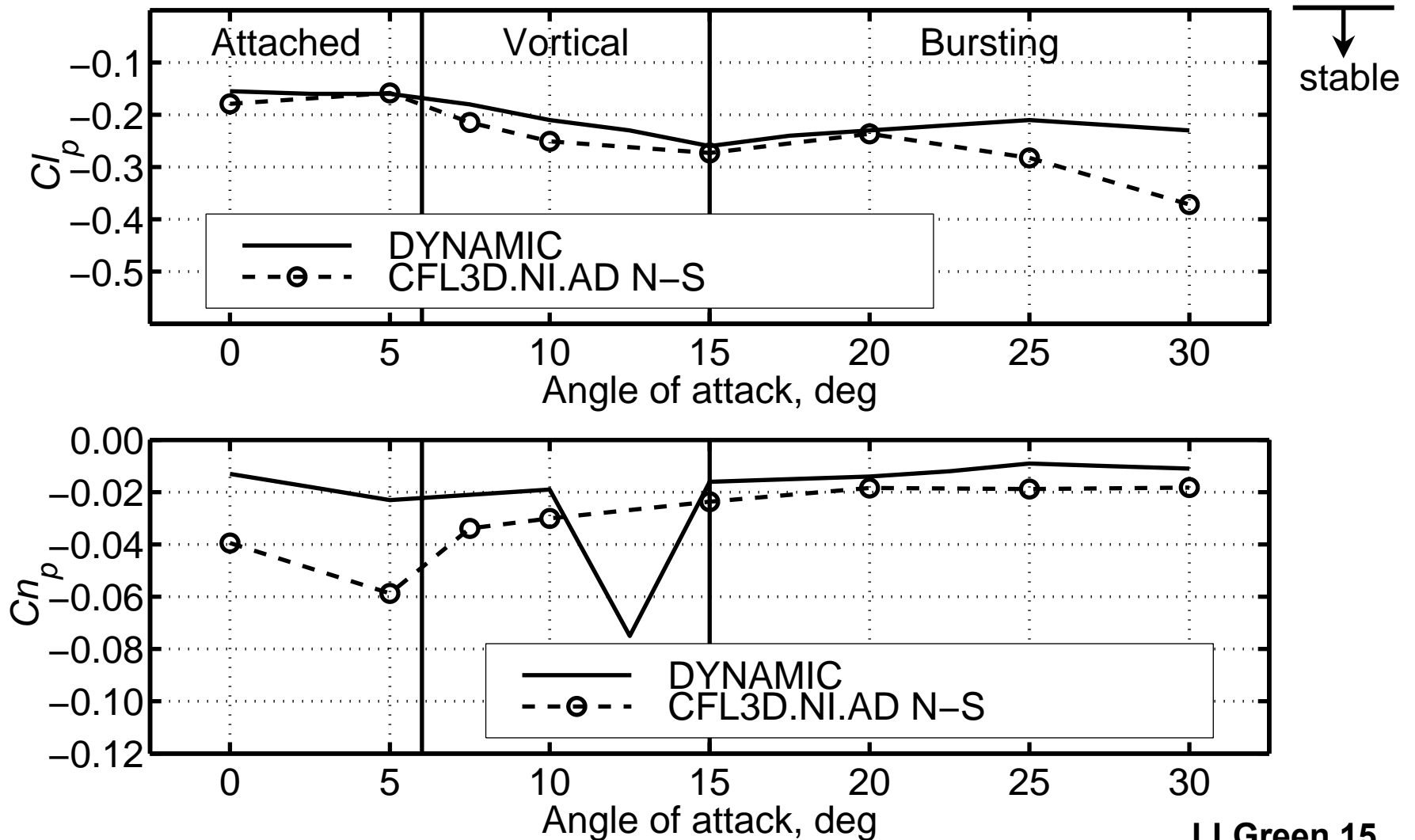
$$\frac{1}{J} = \text{Cell Volume}$$

$$b = \begin{bmatrix} u & v & w \end{bmatrix}$$



# Roll Rate Derivatives

CFL3Dv6.NI.AD N-S / S-A, Mach = 0.6, ICE Configuration



# CFL3D / CFL3D.AD / CFL3D.NI.AD

## Reference Data Comparison Summary, ICE Configuration

Description		Performance in Different Flow Structures		
		Attached	Vortical Bursting	
		0–5 $\alpha$	6–15 $\alpha$	>15 $\alpha$
Force and moment	( <b><math>C_m</math></b> )	Excellent	Excellent	Good
Long. Static stability	( <b><math>C_{m_\alpha}</math></b> )	Excellent	Excellent	Good
Lat. / Dir. Static stability	( <b><math>C_{l_\beta}</math></b> )	Excellent	Good	Poor*
Dynamic derivatives	( <b><math>C_{l_p}</math></b> )	Excellent	Excellent	Good

CFL3D.NI.AD, 0-15 deg  $\alpha$       **30** hr. per angle of attack case

CFL3D.NI.AD, >15 deg  $\alpha$       **90** hr. per angle of attack case

Center-difference CFL3D.NI 0-15 deg  $\alpha$       **44** hr. per angle of attack case

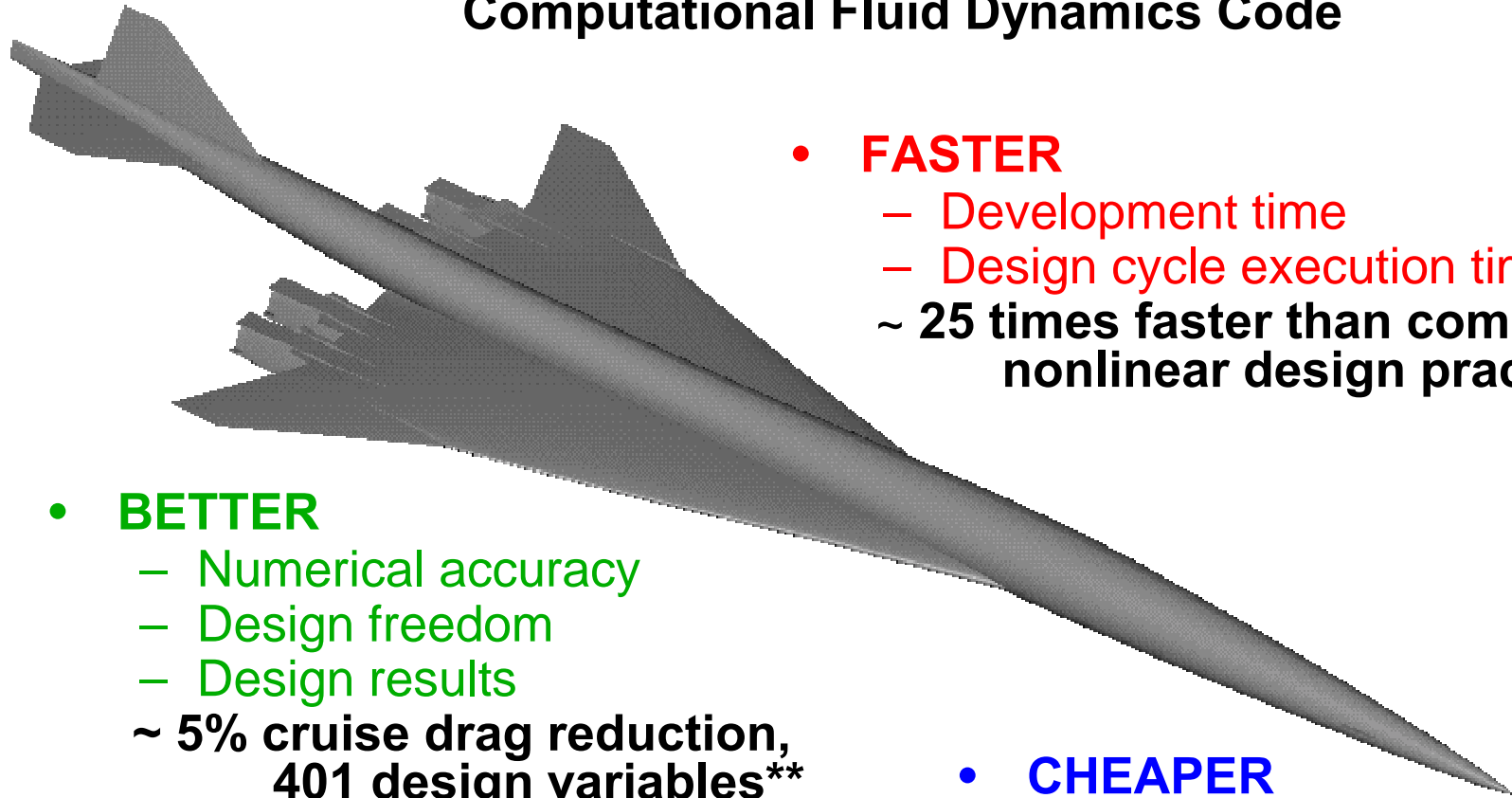
Execution on 16-processor SGI Origin 2000™ with 12 Gb RAM

\* Still better than previous capability



# High Speed Civil Transport Optimization

With ADJIFOR\*-Generated CFL3D Adjoint  
Computational Fluid Dynamics Code



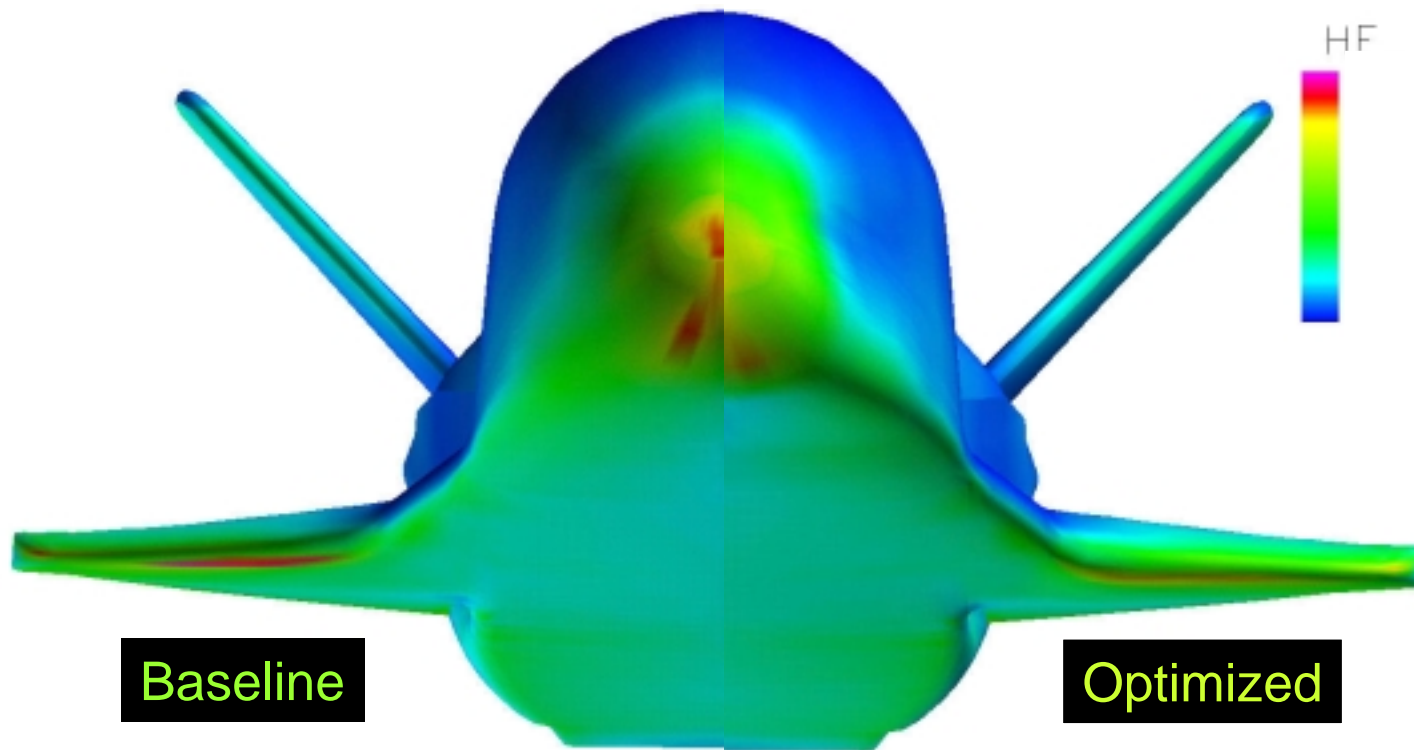
- **FASTER**
  - Development time
  - Design cycle execution time
  - ~ 25 times faster than comparable nonlinear design practice\*\*
- **BETTER**
  - Numerical accuracy
  - Design freedom
  - Design results
  - ~ 5% cruise drag reduction, 401 design variables\*\*
- **CHEAPER**
  - Less human resources
  - Less computer resources
  - ~ 10 times faster inviscid design cycle\*\*

\* Developed by Rice University

\*\* Initial Boeing Long Beach wing-body result

# X-37 Wing/Body Aeroheating Optimization

35 Design Variables to Minimize Maximum Heat Flux  
CFL3D N-S (Menter), 38 Blocks, 0.85M Points

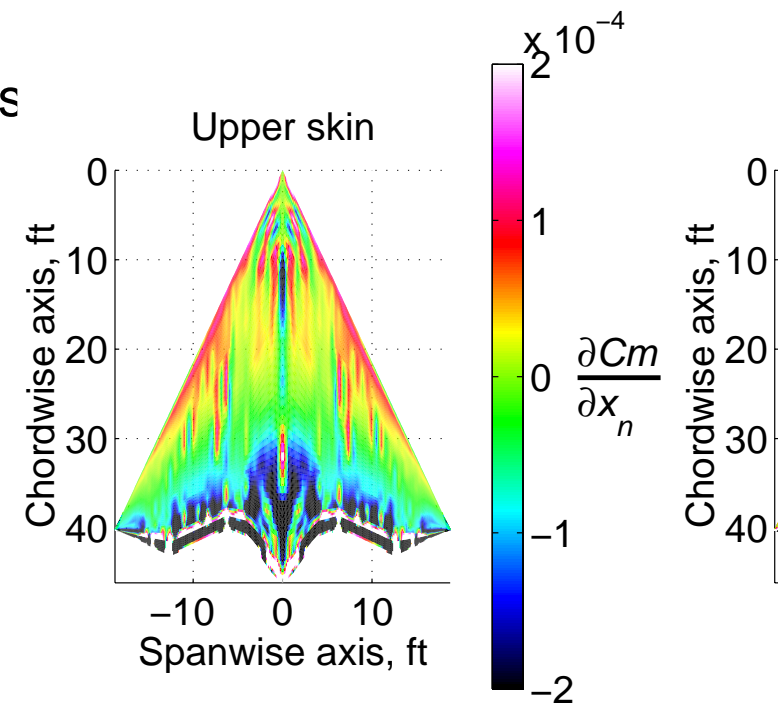
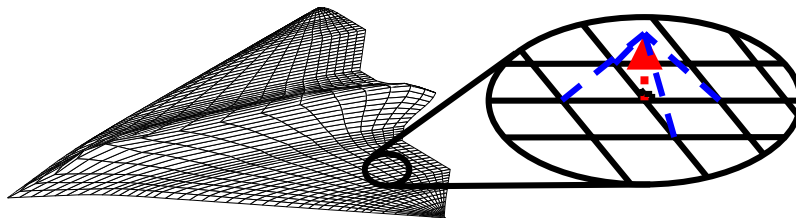


**Max. Heat Flux Reduction  
(7% on Forebody and 16% on Wing Leading-Edge)**

# Control Placement Effectiveness

PMARC.AD linear aerodynamics code

- Model inflatable control effectors as bumps (outward normal displacements ( $X_n$ ) of surface grid points)
- Control placement effectiveness is the **derivative of** pitch ( $C_m$ ), roll ( $C_l$ ), and yaw ( $C_n$ ) moment coefficients **with respect to surface displacement ( $X_n$ )**
- Calculated for each of 1353 surface grid points
- Control effectiveness interpolated over the configuration surface



Part of integrated control effectors design and simulation package presented to NASA Administrator Daniel Goldin

# Ongoing and Future Work

- Non-inertial modifications were implemented in the production version of CFL3Dv6; sensitivity studies of un-commanded aircraft motions (for example, F-18 E/F wing rock) are planned as cooperation between ASCOT and Abrupt Wing Stall Programs
- Second and higher derivative methods are being examined for use with S&C calculations to provide uncertain S&C data on F-16XL for use in robust control law design within ASCOT
- Second and higher derivative methods are being examined for use with aircraft robust design within ASCOT
- First-order sensitivity methods are being applied to the 2<sup>nd</sup> Generation RLV Program for uncertainty quantification and risk reduction
- Sensor / actuator placement studies for deformable nacelles are planned under the Ultra-Efficient Engine Program

# Conclusions

- Automatic Differentiation enables the rapid development of next-generation analysis and design tools from legacy codes
- Automatic Differentiation provides increased confidence through automatic generation of sensitivity analyses
- Automatic Differentiation has contributed significantly to aircraft computational stability and control studies
- Recent MDOB work with ADIFOR has pioneered advanced sensitivity techniques which reduce the computational impact of sensitivity analyses
- MDOB actively seeks to transfer sensitivity tools and techniques to others
- Automatic Differentiation enables probabilistic uncertainty quantification and propagation through method of moments (Newman)

# References 1

- Putko, M. M., Newman, P. A., Taylor III, A. C., and Green, L. L., "Approach for Uncertainty Propagation and Robust Design in CFD Using Sensitivity Derivatives," AIAA Paper 2001-2528, 15th AIAA CFD Conference, Anaheim, CA, June 11-14, 2001.
- Taylor III, A. C., Green, L. L., Newman, P. A., and Putko, M. M., "Some Advanced Concepts in Discrete Aerodynamic Sensitivity Analysis," AIAA Paper 2001-2529, 15th AIAA CFD Conference, Anaheim, CA, June 11-14, 2001.
- Sherman, L., Taylor III, A., Green, L., Newman, P., Hou, G., and Korivi, M., "First- and Second-Order Aerodynamic Sensitivity Derivatives via Automatic Differentiation with Incremental Iterative Methods," Journal of Computational Physics, Vol. 129, No. 2, 1996, pp. 307-336.
- Park, M. A. and Green, L. L.: "Steady-State Computation of Constant Rotational Rate Dynamic Stability Derivatives," AIAA Paper 2000-4321, 18th AIAA Applied Aerodynamics Conference, Denver, CO, August 14-17, 2000.
- Park, M. A.; Green, L. L.; Montgomery, R. C.; and Raney, D. L.: "Determination of Stability and Control Derivatives Using Computational Fluid Dynamics and Automatic Differentiation," AIAA Paper 99-3136, 17th AIAA Applied Aerodynamics Conference, Norfolk, VA, June 28-July 1, 1999.

## References 2

- Limache, A. C., and Cliff, E. M., "Aerodynamic Sensitivity Theory for Rotary Stability Derivatives," AIAA Paper 99-4313, AIAA Atmospheric Flight Mechanics Conference, Portland, OR, August 9-11, 1999.
- Agrawal, S., Narducci, R. P., Kuruvila, G., Sundaram, P., and Hager, J. O.: "CFD-Based Aerodynamic Shape Optimization", European Congress on Computational Methods in Applied Sciences and Engineering, ECCOMAS 2000 Barcelona, September 2000.
- Sundaram, P., Agrawal, S., and Hager, J. O.: "Aerospace Vehicle MDO Shape Optimization Using ADIFOR 3.0 Gradients", AIAA 2000-4733, AIAA/ASME MDO Conference, Long Beach, California, Aug. 2000
- Sundaram, P., Agrawal, S., Hager, J. O., Carle, A., and Fagan, M.: "Viscous Design Optimization Using ADJIFOR - An HPCCP Perspective", NASA HPCCP/CAS Workshop, NASA Ames Research Center, Feb. 2000
- Sundaram, P., and Hager, J. O.: "Applications of Parallel Processing in Aerodynamic Analysis and Design", HPCCP/CAS Workshop, NASA Ames, Aug., 1998.